

Fundamental Kinetics Database Utilizing Shock Tube Measurements

Volume 3: Reaction Rate Measurements

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Abstract

This volume of the *Fundamental Kinetic Database Utilizing Shock Tube Measurements* includes a summary of the reaction rates measured and published by the Hanson Shock Tube Group in the Mechanical Engineering Department of Stanford University. The cut-off date for inclusion in this volume was January 2009.

This work has been supported by many government agencies and private companies including: the U.S. Department of Energy, the Army Research Office, the Office of Naval Research, the Air Force Office of Scientific Research, the National Science Foundation, and the Gas Research Institute.

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Introduction

There is a critical need for standardized experimental data that can be used as targets in the validation and refinement of reaction mechanisms for hydrocarbon fuels. In our laboratory at Stanford University, we are able to provide some of this data in the form of shock tube experiments.

The data from shock tube experiments generally takes three forms: ignition delay times, species concentration time-histories and reaction rate measurements.

Ignition delay times are a measure of the time from initial shock wave heating to a defined ignition point, often a rapid change in pressure or radical species population. These targets place a constraint on the overall predictive behavior of the reaction mechanism. Does the mechanism predict the time of ignition properly for a particular initial temperature, pressure and mixture composition? These ignition delay times can also be provided in the form of correlation equations which provide similar information in a compact form.

Species concentration time-histories are a measure of the concentration of a particular species as a function of time during the entire experiment. These targets place strong constraints on the internal workings of the reaction mechanism. Concentration time-histories for OH, for example, are strongly related to the concentrations of other small radical species including: H-atoms, O-atoms, and HO₂. The production and removal rates of these species have an important role in the reaction progress to ignition.

Reaction rate measurements provide the basic rate data that reaction mechanisms are comprised of. Accurate measurements are needed of the rates of critical reactions that important reaction parameters are sensitive to, such as ignition delay times, heat release rates, and product species. These are necessary as it is not yet possible to accurately predict these rates (nor is it likely that they will ever be reliably predicted) without experimental verification.

Shock tube data are well suited for comparison with computation models. Shock wave experiments can provide near constant-volume test conditions, generally over the entire time period before ignition, and in many cases for longer times. Shock tube experiments can provide test conditions over a wide range of temperatures, pressure and gas mixtures, typically over temperatures of 600 to 4000 K, pressures from sub-atmospheric to 1000 atm, and fuel concentrations from ppm to percent levels with test times in the 1-10 ms range. Methods have been developed to extend these ranges if need be. The nature of planar shock wave flows as they are formed in conventional shock tubes means that the test gas mixtures are effectively instantaneously compressed and heated, providing very simple initial conditions for modeling. The spatial uniformity of the stationary

heated test gas mixture behind reflected shock waves means that only chemistry need be modeled, and fluid mechanical effects such as diffusion, mixing, and fluid movement are not significant in most cases. And finally, the time scales and physical dimensions of shock tube experiments means that the test gas volume can be considered to be adiabatically isolated from its surroundings.

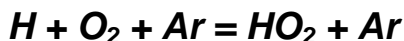
The database is comprised of three volumes: Volume 1, ignition delay time measurements; Volume 2, species concentration time-histories; and Volume 3, reaction rate measurements. The formal cut-off point for Volume 3 is January 2009, and work published after this data will be included in later editions.

A version of the database is available through the PRIME warehouse currently being developed at University of California, Stanford University and NIST.

Database Format

In this report temperatures are given in Kelvin and activation energies are given in calories/mole and using $R = 1.987$ [mole/calories/K] when a conversion from a published activation energy in Kelvins is needed and 4.18 Joules = 1 calorie when the published activation energy is in Joules. Reaction rate constants are given in units of $[1/s]$, $[cm^3/mol/s]$, or $[cm^6/mol^2/s]$. Pressures are quoted in atm or bar. The publications are listed in approximately reverse chronological order.

Dissociation/Association Reactions



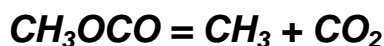
G. A. Pang, D. F. Davidson, R. K. Hanson, "Experimental Study and Modeling of Shock Tube Ignition Delay Times for Hydrogen-Oxygen-Argon Mixtures at Low Temperatures," Proceedings of the Combustion Institute 32 (2009) 181-188.

For 908-1118 K, 3.0-3.8 atm:

$$k_{\infty} = 1.04 \times 10^{13} T^{0.2} \text{ [cm}^3\text{/mol/s];}$$

$$k_0 = 6.99 \times 10^{18} T^{-1.2} \text{ [cm}^6\text{/mol}^2\text{/s]}, F_{\text{cent}} = 0.7.$$

This study provides a preliminary measurement of this rate in this temperature range.

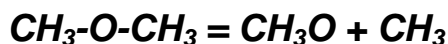


A. Farooq, D. F. Davidson, R. K. Hanson, L. K. Huynh, A. Violi, "An Experimental and Computational Study of Methyl Ester Decomposition Pathways using Shock Tubes," Proceedings of the Combustion Institute 32 (2009) 247-253.

For 1260-1653 K, 1.4-1.7 atm:

$$k = 1.55 \times 10^{12} T^{0.514} \exp(-15182/RT) \text{ [1/s].}$$

This study provides a confirmation of the reaction rate suggested by L. K. Huynh, A. Violi, J. Org. Chem. 73 (2008) 94-101.

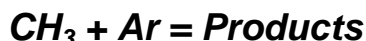


R. D. Cook, D. F. Davidson, R. K. Hanson, "Shock Tube Measurements of Ignition Delay Times and OH Time-Histories in Dimethyl Ether Oxidation," Proceedings of the Combustion Institute 32 (2009) 189-196.

For 680-1750 K, 1.6-6.6 bar:

$$k = 1.61 \times 10^{79} T^{-18.4} \exp(116438/RT) \text{ [1/s]}$$

This rate was inferred based on this and previous studies.



V. Vasudevan, R. K. Hanson D. M. Golden, C. T. Bowman, D. F. Davidson, "High-Temperature Shock Tube Measurements of Methyl Radical Decomposition," Journal Physical Chemistry A 111 (2007) 4062-4072.

For 2706-3527 K, 0.7-4.2 atm:

$$k = 3.09 \times 10^{15} \exp(-80871/RT) \text{ [cm}^3\text{/mol/s] for the CH+H}_2 \text{ channel}$$

For 2253-2975 K, 1.1-3.9 atm:

$$k = 2.24 \times 10^{15} \exp(-82659/RT) \text{ [cm}^3\text{/mol/s] rate for the CH}_2\text{+H channel}$$

This study also includes the rate for the CH+H₂ channel.



M. A. Oehlschlager, D. F. Davidson, R. K. Hanson, "Thermal Decomposition of Toluene: Overall Rate and Branching Ratio," Proceedings of the Combustion Institute 31 (2007) 211-219. See also Western States Section/Combustion Institute Fall 2005 Meeting, October 17-18, 2005, paper 05F-59.

For 1400-1780 K, 1.5 bar:

$k = 2.09 \times 10^{15} \exp(-87510/RT)$ [$\text{cm}^3/\text{mol/s}$] for the $\text{C}_6\text{H}_5\text{CH}_2 + \text{H}$ channel.

$k = 2.66 \times 10^{16} \exp(-97880/RT)$ [$\text{cm}^3/\text{mol/s}$] for the $\text{C}_6\text{H}_5 + \text{CH}_3$ channel.

***n*-C₇H₁₆ = Products**

D. F. Davidson, M. A. Oehlschlaeger, R. K. Hanson, "Methyl Concentration Time-Histories during Iso-Octane and N-Heptane Oxidation and Pyrolysis," Proceedings of the Combustion Institute 31 (2007) 321-328. See also Western States Section/Combustion Institute Fall 2005 Meeting, October 17-18, 2005, paper 05F-61.

For 1300-1690 K, 1.8 atm:

$k = 9.00 \times 10^{14} \exp(-67300/RT)$ [1/s]

This study also includes the rate for iso-octane decomposition.

***iso*-C₈H₁₈ = Products**

D. F. Davidson, M. A. Oehlschlaeger, R. K. Hanson, "Methyl Concentration Time-Histories during Iso-Octane and N-Heptane Oxidation and Pyrolysis," Proceedings of the Combustion Institute 31 (2007) 321-328. See also Western States Section/Combustion Institute Fall 2005 Meeting, October 17-18, 2005, paper 05F-61.

For 1200-1400 K, 1.7 atm:

$k = 5.20 \times 10^{15} \exp(-67800/RT)$ [1/s]

This study also includes the rate for n-heptane decomposition.

***CH*₂O + Ar = Products**

V. Vasudevan, D. F. Davidson, R. K. Hanson, C. T. Bowman, D. M. Golden, "High-Temperature Measurements of the Rates of the Reactions *CH*₂O+Ar=Products and *CH*₂O+O₂=Products," Proceedings of the Combustion Institute 31 (2007) 175-183. See also Western States Section/Combustion Institute Fall 2005 Meeting, October 17-18, 2005, paper 05F-40.

For 2258-2687 K, 1.6 atm:

$k = 5.85 \times 10^{14} \exp(-63783/RT)$ [$\text{cm}^3/\text{mol/s}$] *HCO*+*H* channel

$k = 4.64 \times 10^{14} \exp(-57027/RT)$ [$\text{cm}^3/\text{mol/s}$] *H*₂+*CO* channel

This study also includes rate measurements of *CH*₂O+O₂.

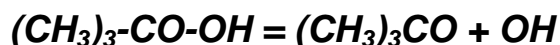
***C*₆*H*₅*CH*₂ = Products**

M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "High-Temperature Thermal Decomposition of Benzyl Radicals," Journal Physical Chemistry A 110 (2006) 6649-6653.

For 1430-1730 K, 1.5 bar:

$k = 8.20 \times 10^{14} \exp(-80672/RT)$ [1/s]

This study assumes the products are *C*₇*H*₆+*H*.



V. Vasudevan, D. F. Davidson, R. K. Hanson, "Direct Measurements of the Reaction of $OH+CH_2O=HCO+H_2O$ at High Temperatures," International Journal of Chemical Kinetics 37 (2005) 98-109.

For 900-1000 K, 1.6 bar:

$$k = 2.50 \times 10^{15} \exp(-43000/RT) \text{ [cm}^3/\text{mol/s]}$$

This study also includes a measurement of the reaction of CH_2O+OH .

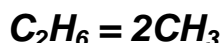


M. A. Oehlschlaeger, D. F. Davidson, J. B. Jeffries, R. K. Hanson, "Carbon Dioxide Thermal Decomposition: Observation of Incubation," Z. Phys. Chem. 219 (2005) 555-567.

For 3200-4600 K, 45-100 kPa:

$$k = 3.14 \times 10^{14} \exp(-101933/RT) \text{ [cm}^3/\text{mol/s]}$$

This study includes a determination of the incubation time for this reaction.



M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "High-Temperature Ethane and Propane Decomposition," Proceedings of the Combustion Institute 30 (2005) 1119-1127. See also Western States Section/Combustion Institute Fall 2003 Meeting October 20-21, 2003, Paper 03F-56.

For 700-1924 K, 0.13-8.4 atm, in argon:

$$k_{\infty} = 1.88 \times 10^{50} T^{-9.72} \exp(-107338/RT) \text{ [1/s];}$$

$$k_0 = 3.72 \times 10^{65} T^{-13.14} \exp(-101575/RT) \text{ [cm}^3/\text{mol/s];}$$

$$F_{\text{cent}} = 0.61 \exp(-T/100K) + 0.39 \exp(-T/1900K) + \exp(-6000K/T).$$

This study includes a determination of the propane decomposition rate also.



M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "High-Temperature Ethane and Propane Decomposition," Proceedings of the Combustion Institute 30 (2005) 1119-1127. See also Western States Section/Combustion Institute Fall 2003 Meeting October 20-21, 2003, Paper 03F-56.

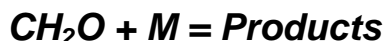
For 600-1653 K, 0.13-8.4 atm in argon:

$$k_{\infty} = 1.29 \times 10^{37} T^{-5.84} \exp(-97383/RT) \text{ [1/s];}$$

$$k_0 = 5.64 \times 10^{74} T^{-15.74} \exp(-98714/RT) \text{ [cm}^3/\text{mol/s];}$$

$$F_{\text{cent}} = 0.69 \exp(-T/50K) + 0.31 \exp(-T/3000K) + \exp(-9000K/T).$$

This study includes a determination of the ethane decomposition rate also.



G. Friedrichs, D. F. Davidson, R. K. Hanson, "Validation of a Thermal Decomposition Mechanism of Formaldehyde by Detection of CH_2O and HCO behind Shock Waves," International Journal of Chemical Kinetics 36 (2004) 157-169.

For 1675-2080 K, 1 bar:

$$k = 3.3 \times 10^{39} T^{-6.3} \exp(-100000/RT) \text{ [cm}^3/\text{mol/s]} \text{ for the } H+HCO \text{ channel.}$$

$k = 3.1 \times 10^{45} T^{-8.0} \exp(-97608/RT)$ [cm³/mol/s] for the H₂+CO channel.
 These rates are based on RRKM fits to the current study's data. A reaction rate for CH₂OH+HCO is all provided in this study.

Iso-C₄H₁₀ = CH₃ + i-C₃H₇

M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "High-Temperature Thermal Decomposition of Iso-Butane and n-Butane Behind Shock Waves," Journal Physical Chemistry A 108 (2004) 4247-4253. See also Western States Section/Combustion Institute Fall 2003 Meeting October 20-21, 2003, Paper 03F-56.

For 1320-1560 K, 0.20-8.8 atm, in argon:

$$k_{\infty} = 4.83 \times 10^{16} \exp(-79897/RT) [1/s];$$

$$k_0 = 2.41 \times 10^{14} \exp(-52576/RT) [cm^3/mol/s];$$

$$F_{cent} = 0.75 \exp(-T/750K).$$

This study includes a determination of the n-butane decomposition rate also.

n-C₄H₁₀ = Products

M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "High-Temperature Thermal Decomposition of Iso-Butane and n-Butane Behind Shock Waves," Journal Physical Chemistry A 108 (2004) 4247-4253. See also Western States Section/Combustion Institute Fall 2003 Meeting October 20-21, 2003, Paper 03F-56.

For 1320-1600 K, 0.20-8.8 atm, in argon:

$$k_{\infty} = 4.28 \times 10^{14} \exp(-69903/RT) [1/s];$$

$$k_0 = 5.34 \times 10^{17} \exp(-42956/RT) [cm^3/mol/s];$$

$$F_{cent} = 0.28 \exp(-T/1500K) \text{ for the } CH_3+n-C_3H_7 \text{ channel.}$$

$$k_{\infty} = 2.72 \times 10^{15} \exp(-75605/RT) [1/s];$$

$$k_0 = 4.72 \times 10^{18} \exp(-49576/RT) [cm^3/mol/s];$$

$$F_{cent} = 0.28 \exp(-T/1500K) \text{ for the } C_2H_5+C_2H_5 \text{ channel.}$$

This study includes a determination of the iso-butane decomposition rate also.

HCO + M = H + CO + M

G. Friedrichs, J. T. Herbon, D. F. Davidson, R. K. Hanson, "Quantitative Detection of HCO behind Shock Waves: The Thermal Decomposition of HCO," Physical Chemistry Chemical Physics 4 (2002) 5778-5788.

For 835-1230 K and near 1 bar:

$$k = 4.0 \times 10^{13} \exp(-15550/RT) [cm^3/mol/s].$$

This study includes and RRKM fit to this rate, as well as determinations of the rate of H+HCO and HCO+HCO.

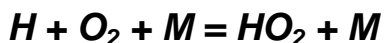
C₆H₅CH₂NH₂ = NH₂ + C₆H₅CH₂

S. Song, D. M. Golden, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Benzylamine Decomposition: Overall Rate Coefficient and Heat of Formation of the Benzyl Radical," Journal Physical Chemistry A 106 (2002) 6094-6098.

For 1225-1599 K, 1.19-1.47 bar:

$k = 5.49 \times 10^{14} \exp(-65790/RT)$ [cm³/mol/s].

A high-pressure-limit rate is also provided in this study.



R. W. Bates, D. M. Golden, R. K. Hanson, C. T. Bowman, "Experimental Study and Modeling of the Reaction $H+O_2+M=HO_2+M$ ($M = Ar, N_2, H_2O$) at Elevated Pressures and Temperatures between 1050 and 1250 K," Physical Chemistry Chemical Physics 3 (2001) 2337-2342. See also Joint U. S. Sections Technical Meeting, The Combustion Institute, Washington DC, March 1999, Abstract book pp. 629-632.

For 1050-1250 K, 7-152 bar:

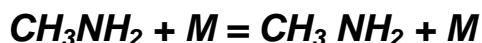
$k_{\infty} = 9.04 \times 10^{12} T^{0.2}$ [cm³/mol/s];

$k_0 = 6.80 \times 10^{18} T^{-1.2}$ [cm⁶/mol²/s] for Ar:

$k_0 = 2.65 \times 10^{19} T^{-1.3}$ [cm⁶/mol²/s] for N₂:

$k_0 = 3.70 \times 10^{19} T^{-1.0}$ [cm⁶/mol²/s] for H₂O:

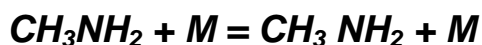
$F_{cent} = 0.7$ for Ar and N₂ and $F_{cent} = 0.8$ for H₂O.



M. Votsmeier, S. Song, D. F. Davidson, R. K. Hanson, "Shock Tube Study of Monomethylamine Thermal Decomposition and NH₂ High Temperature Absorption Coefficient," International Journal of Chemical Kinetics 31 (1999) 323-330.

For 1550-1900 K, 1.6 atm:

$k = 2.51 \times 10^{15} \exp(-56490/RT)$ [cm³/mol/s].

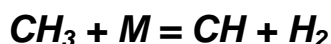


M. Votsmeier, S. Song, D. F. Davidson, R. K. Hanson, "Sensitive Detection of NH₂ in Shock Tube Experiments Using Frequency Modulation Spectroscopy," International Journal of Chemical Kinetics 31 (1999) 323-330. . See also Joint U. S. Sections Technical Meeting, The Combustion Institute, Washington DC, March 1999. Abstract book pp. 645-648.

For 1530-1975 K, 1.3 atm:

$k = 8.17 \times 10^{16} \exp(-61020/RT)$ [cm³/mol/s].

A related study using conventional absorption spectroscopy is found in M. Votsmeier, S. Song, D. F. Davidson, R. K. Hanson, International Journal of Chemical Kinetics 31 (1999) 323-330.



M. Roehrig, E. L. Petersen, D. F. Davidson, R. K. Hanson, C. T. Bowman, "Measurement of the Rate Coefficient of the Reaction $CH+O_2=Products$ in the Temperature Range 2200 to 2600 K," International Journal of Chemical Kinetics 29 (1997) 781-789.

For 2200-2600 K, 1.3 atm:

$k = 1.00 \times 10^{16} \exp(-85242/RT)$ [cm³/mol/s].

This study also includes a determination of the rate of $CH+O_2$ and CH_2+H .



M. Roehrig, E. L. Petersen, D. F. Davidson, R. K. Hanson, "A Shock Tube Study of the Pyrolysis of NO_2 ," International Journal of Chemical Kinetics 29 (1997) 483-493. See also Western States Section/The Combustion Institute 1995 Fall Meeting, Stanford University, October 30-31, 1995, paper 95F-156.

For 1350-2100 K, 42-380 atm, for argon:

$$k_{\infty} = 3.98 \times 10^{14} \exp(-71770/RT) \text{ [1/s];}$$

$$k_0 = 3.98 \times 10^{15} \exp(-60048/RT) \text{ [cm}^3\text{/mol/s] for Ar:}$$

This study also includes a determination of the reaction rate of $\text{NO}_2 + \text{NO}_2$.

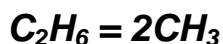


M. Roehrig, E. L. Petersen, D. F. Davidson, R. K. Hanson, "The Pressure Dependence of the Thermal Decomposition of N_2O ," International Journal of Chemical Kinetics 28 (1996) 599-608.

For 1570-3100 K, 0.3-450 atm, for argon:

$$k_{\infty} = 1.26 \times 10^{12} \exp(-56700/RT) \text{ [1/s];}$$

$$k_0 = 3.98 \times 10^{14} \exp(-62679/RT) \text{ [cm}^3\text{/mol/s].}$$



D. F. Davidson, R. K. Hanson, C. T. Bowman, "Communication: Revised Values of the Rate Coefficients of Ethane and Methane Decomposition," International Journal of Chemical Kinetics 27 (1995) 305-308.

For 1450-1945 K, 1 atm, for argon:

$$k = 7.94 \times 10^{11} \exp(-60206/RT) \text{ [1/s].}$$

This paper provides a reaction rate for methane decomposition as well.

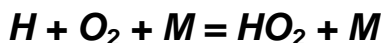


D. F. Davidson, R. K. Hanson, C. T. Bowman, "Communication: Revised Values of the Rate Coefficients of Ethane and Methane Decomposition," International Journal of Chemical Kinetics 27 (1995) 305-308.

For 1785-2325 K, 1 atm, for argon:

$$k = 1.04 \times 10^{18} \exp(-96389/RT) \text{ [1/s].}$$

This paper provides a reaction rate for ethane decomposition as well.



D. F. Davidson, E. L. Petersen, M. Roehrig, R. K. Hanson, "Measurement of the Rate Coefficient of $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$ for $\text{M} = \text{Ar}$ and N_2 at High Pressures," Proceedings of the Combustion Institute 26 (1996) 481-488.

For 1260-1375 K, 50-115 atm:

$$k_0 = 7.0 \times 10^{17} T^{-0.8} \text{ [cm}^6\text{/mol}^2\text{/s] for M = Ar;}$$

$$k_0 = 2.6 \times 10^{19} T^{-1.24} \text{ [cm}^6\text{/mol}^2\text{/s] for M = N}_2\text{.}$$



M. S. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Nitric Acid Decomposition," Proceedings of the 19th International Symposium on Shock Waves, Marseille, France, July 26-30, 1993, Vol. II, pp. 83-88.

For 1120-1960 K, 0.15-1.01 atm:

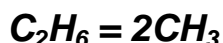
$$k = 1.01 \times 10^{16} \exp(-34335/RT) \text{ [cm}^3/\text{mol/s]}.$$



L. S. Zelson, D. F. Davidson, R. K. Hanson, "V.U.V. Absorption Diagnostic for Shock Tube Kinetics Studies of C₂H₄," Journal Quantitative Spectroscopy and Radiative Transfer 52 (1994) 31-43. See also Western States Section/The Combustion Institute 1993 Fall Meeting, Menlo Park CA, October 18-19, 1993, Paper 93-057.

For 1600-2300 K, 1.2 atm:

$$k = 9.17 \times 10^{16} \exp(-75069/RT) \text{ [cm}^3/\text{mol/s]}.$$



D. F. Davidson, M. D. Di Rosa, R. K. Hanson, C. T. Bowman, "A Study of Ethane Decomposition in a Shock Tube using Laser Absorption of CH₃," International Journal of Chemical Kinetics 25 (1993) 969-982.

For 1350-2110 K, 0.58-4.4 atm:

Measurement results were corrected in D. F. Davidson, R. K. Hanson, C. T. Bowman, Internat. J. Chem. Kinet. 27 (1995) 305-308.



D. F. Davidson, M. D. Di Rosa, A. Y. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Methane Decomposition using Laser Absorption of CH₃," Proceedings of the Combustion Institute 24 (1992) 589-596.

For 1790-2325 K, 0.56-3.76 atm:

Measurement results were corrected in D. F. Davidson, R. K. Hanson, C. T. Bowman, Internat. J. Chem. Kinet. 27 (1995) 305-308.



D. F. Davidson, K. Kohse-Hoeinghaus, A. Y. Chang, R. K. Hanson, , "A Pyrolysis Mechanism for Ammonia," International Journal of Chemical Kinetics 22 (1990) 513-535. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-95.

For 2200-2800 K, 0.8-1.1 atm:

$$k = 2.2 \times 10^{16} \exp(-93470/RT) \text{ [cm}^3/\text{mol/s]}.$$

Reaction rates for NH₂+H, NH₂+NH, and NH₂+NH₂ are also included in this paper.



J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "Reaction Kinetics of NH in the Shock Tube Pyrolysis of HNCO," International Journal of Chemical

Kinetics 21 (1989) 1049-1067. See also Western States Section/ The Combustion Institute 1988 Fall Meeting, Dana Point CA October 17-18, 1988, Paper 88-64.

For 1830-3340 K, 0.3-2.1 atm:

$$k = 9.84 \times 10^{15} \exp(-85441/RT) \text{ [cm}^3/\text{mol/s]}.$$

This paper provides reaction rates for NH+NH and NH+Ar as well.

$NH + Ar = N + HAr$

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "Reaction Kinetics of NH in the Shock Tube Pyrolysis of HNCO," International Journal of Chemical Kinetics 21 (1989) 1049-1067. See also Western States Section/ The Combustion Institute 1988 Fall Meeting, Dana Point CA October 17-18, 1988, Paper 88-64.

For 3140-3320 K, 0.3-2.1 atm:

$$k = 2.65 \times 10^{14} \exp(-75506/RT) \text{ [cm}^3/\text{mol/s]}.$$

This paper provides reaction rates for HNCO+Ar and NH+NH as well.

$NCO + M = N + CO + M$

M. Y. Louge, R. K. Hanson, "High Temperature Kinetics of NCO," Combustion and Flame 58 (1984) 291-300.

For 2150-2400 K, 0.6 atm:

$$k = 6.3 \times 10^{16} T^{-0.5} \exp(-47688/RT) \text{ [cm}^3/\text{mol/s]}.$$

Rates are also presented for NCO+H and NCO+H₂.

$HCN + Ar = H + CN + Ar$

A. Szekely, R. K. Hanson, C. T. Bowman, "Thermal Decomposition of Hydrogen Cyanide behind Incident Shock Waves," Journal Physical Chemistry 88 (1984) 666-668.

For 2700-3600 K, 0.6 atm:

$$k = 1.0 \times 10^{16} \exp(-108589/RT) \text{ [cm}^3/\text{mol/s]}.$$

$C_2N_2 + Ar = 2CN + Ar$

A. Szekely, R. K. Hanson, C. T. Bowman, "Shock Tube Study of the Thermal Decomposition of Hydrogen Cyanogen," Journal Physical Chemistry 80 (1984) 4982-4985.

For 2500-3450 K, 0.23-58 bar:

$$k = 6.3 \times 10^{16} \exp(-99429/RT) \text{ [cm}^3/\text{mol/s]}.$$

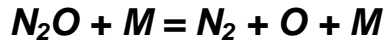
$NH_3 + M = NH_2 + H + M$

T. R. Roose, R. K. Hanson, C. H. Kruger, "Thermal Decomposition of NH₃ in Shock Waves," Proceedings of the 12th International Symposium on Shock Tubes and Waves (1980) pp. 476-485.

For 2200-3450 K, 0.14-0.6 atm:

$$k = 2.52 \times 10^{16} \exp(-93786/RT) \text{ [cm}^3/\text{mol/s]}.$$

Rates for the NH+H₂ product channel are also provided in this paper.



W. L Flower, R. K. Hanson, C. H Kruger, "*Experimental Study of Nitric Oxide Decomposition by Reaction with Hydrogen,*" Combustion, Science and Technology 15 (1977) 115-128.

For 1815-3365 K, 0.6 atm:

$$k = 1.42 \times 10^{14} \exp(-51280/RT) \text{ [cm}^3\text{/mol/s]}.$$

A rate for $\text{N}_2\text{O} + \text{O}$ is also presented in this paper.

Bimolecular Reactions

2007-2008

CH₃OH + OH = Products

V. Vasudevan, R. D. Cook, R. K. Hanson, C. T. Bowman, D. M. Golden, *"High-Temperature Shock Tube Study of the Reactions CH₃+OH = Products and CH₃OH+Ar = Products,"* International Journal of Chemical Kinetics 40 (2008) 488-495.

For 1904-2298 K, 1.21-1.41 atm:

No rate expression given; data table provided. Measurements are in agreement with experiments of N. K. Srinivasan, M.-C. Su, J. V. Michael, J. Phys. Chem. A 111 (2007) 3951-3958 and theory of A. W. Jasper, S. J. Klippenstein, L. B. Harding, B. Ruscis, J. Phys. Chem. A 111 (2007) 3932-3950..

CH₃ + OH = Products

V. Vasudevan, R. D. Cook, R. K. Hanson, C. T. Bowman, D. M. Golden, *"High-Temperature Shock Tube Study of the Reactions CH₃+OH = Products and CH₃OH+Ar = Products,"* International Journal of Chemical Kinetics 40 (2008) 488-495.

For 1081-1426 K, 1.21-4.95 atm:

No rate expression given; data table provided. Measurements are in agreement with theory of A. W. Jasper, S. J. Klippenstein, L. B. Harding, B. Ruscis, J. Phys. Chem. A 111 (2007) 3932-3950.

CH + N₂ = Products

V. Vasudevan, R. K. Hanson, C. T. Bowman, D. M. Golden, D. F. Davidson, *"Shock Tube Study of the Reaction of CH with N₂: Overall Rate and Branching Ratio,"* Journal Physical Chemistry A 111 (2007) 11818-11830.

For 1943-3543 K, 0.9-1.4 atm:

$k = 6.03 \times 10^{12} \exp(-22155/RT)$ [cm³/mol/s]

This study includes evidence of the NCN+H channel.

CH₂O + O₂ = Products

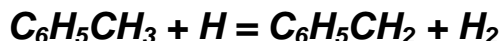
V. Vasudevan, D. F. Davidson, R. K. Hanson, C. T. Bowman, D. M. Golden, *"High-Temperature Measurements of the Rates of the Reactions CH₂O+Ar=Products and CH₂O+O₂=Products,"* Proceedings of the Combustion Institute 31 (2007) 175-183. See also Western States Section/Combustion Institute Fall 2005 Meeting, October 17-18, 2005, paper 05F-40.

For 1480-2367 K, 0.91-1.96 atm:

$k = 5.08 \times 10^{14} \exp(-46297/RT)$ [cm³/mol/s]

This study also includes rate measurements of CH₂O+Ar.

2005-2006

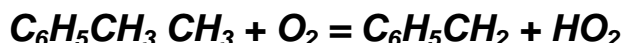


M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "Experimental Investigation of Toluene+H = Benzyl+H₂ at High Temperatures," Journal Physical Chemistry A 110 (2006) 9867-9873.

For 1256-1667 K, 1.7 bar:

$$k = 1.33 \times 10^{15} \exp(-14880/RT) \text{ [cm}^3/\text{mol/s]}$$

This study provides a non-Arrhenius fit to this data and the lower temperature data C. Ellis, M. S. Scott, R. W. Walker, Combust. Flame 132 (2003) 291.



M. A. Oehlschlaeger, D. F. Davidson, R. K. Hanson, "Investigation of the Reaction of Toluene with Molecular Oxygen in Shock-Heated Gases," Combustion and Flame 147 (2006) 195-208.

For 1117-1366 K, 1.7 bar:

$$k = 2.18 \times 10^7 T^{2.5} \exp(-46045/RT) \text{ [cm}^3/\text{mol/s]}$$

This reaction rate determination includes data from the lower temperature study of T. Ingham, R. W. Walker, R. E. Woolford, Proc. Combust. Inst. 25 (1994) 767-774.



V. Vasudevan, D. F. Davidson, R. K. Hanson, "Direct Measurements of the Reaction of OH+CH₂O=HCO+H₂O at High Temperatures," International Journal of Chemical Kinetics 37 (2005) 98-109. See also Joint Meeting of the U.S. Sections of the Combustion Institute, Philadelphia PA, March 22, 2005, Paper C23.

For 934-1670 K, 1.6 bar:

$$k = 7.82 \times 10^7 T^{1.63} \exp(1055/RT) \text{ [cm}^3/\text{mol/s]}$$

This reaction rate determination includes data from the lower temperature study of V. Sivakumaran, D. Holscher, T. J. Dillon, J. N. Crowley, Phys. Chem. Chem. Phys. 5 (2003) 4821-4827.



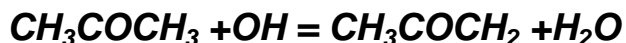
V. Vasudevan, D. F. Davidson, R. K. Hanson, "High-Temperature Measurements of the Reactions of OH with Toluene and Acetone," Journal of Physical Chemistry A 109 (2005) 3352-3359. See also the 25th International Symposium on Shock Waves, Bangalore India, July 2005. See also Joint Meeting of the U.S. Sections of the Combustion Institute, Philadelphia PA, March 22, 2005, Paper C23.

For 570-1389 K, 2.25 bar:

$$k = 1.62 \times 10^{13} \exp(-2770/RT) \text{ [cm}^3/\text{mol/s]}$$

This reaction rate determination includes data from the lower temperature study of F. P. Tully, A. R. Ravishankara, R. L. Thomson, J. M. Nicovich, R. C. Shah, N.

M. Kreutter, P. H. Wine, J. Phys. Chem. 85 (1981) 2262-2269. See also International

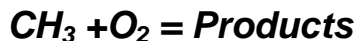


V. Vasudevan, D. F. Davidson, R. K. Hanson, "High-Temperature Measurements of the Reactions of OH with Toluene and Acetone," Journal of Physical Chemistry A 109 (2005) 3352-3359. See also Joint Meeting of the U.S. Sections of the Combustion Institute, Philadelphia PA, March 22, 2005, Paper C23.

For 982-1300 K, 1.65 bar:

$$k = 2.95 \times 10^{13} \exp(-4564/RT) \text{ [cm}^3\text{/mol/s]}$$

This study also includes a measurement of the rate of toluene+OH.



J. T. Herbon, R. K. Hanson, C. T. Bowman, D. M. Golden, "The Reaction of $\text{CH}_3 + \text{O}_2$: Experimental Determination of the Rate Coefficients for the Product Channels at High Temperatures" Proceedings of the Combustion Institute 30 (2005) 955-963.

For 1590-2430 K, 1.4 atm:

$$k = 6.08 \times 10^7 T^{1.54} \exp(-27828/RT) \text{ [cm}^3\text{/mol/s]} \text{ for the } \text{CH}_3\text{O} + \text{O channel.}$$

$$k = 68.6 T^{2.86} \exp(-9768/RT) \text{ [cm}^3\text{/mol/s]} \text{ for the } \text{CH}_2\text{O} + \text{OH channel.}$$

2000-2004

$\text{CH}_2\text{OH} + \text{HCO} = 2\text{CH}_2\text{O}$

G. Friedrichs, D. F. Davidson, R. K. Hanson, "Validation of a Thermal Decomposition Mechanism of Formaldehyde by Detection of CH_2O and HCO behind Shock Waves," International Journal of Chemical Kinetics 36 (2004) 157-169.

For 1710-2100 K, 1 bar:

$$k = 1.5 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

A reaction rate for $\text{CH}_2\text{O} + \text{M}$ is all provided in this study.

$\text{NH}_2 + \text{CH}_4 = \text{NH}_3 + \text{CH}_3$

S. Song, D. M. Golden, R. K. Hanson, C. T. Bowman, J. P. Senosianin, C. B. Musgrave, G. Friedrichs, "A Shock Tube Study of the Reaction $\text{NH}_2 + \text{CH}_4 = \text{NH}_3 + \text{CH}_3$ and Comparison with Transition State Theory," International Journal of Chemical Kinetics 35 (2003) 304-309.

For 1591-2084 K, 1.10-1.33 bar:

$$k = 1.47 \times 10^3 T^{3.01} \exp(-9934/RT) \text{ [cm}^3\text{/mol/s]}.$$

This rate is based on the experiment and TST theory.

$\text{H} + \text{HCO} = \text{H}_2 + \text{CO}$

G. Friedrichs, J. T. Herbon, D. F. Davidson, R. K. Hanson, "Quantitative Detection of HCO behind Shock Waves: The Thermal Decomposition of HCO ," Physical Chemistry Chemical Physics 4 (2002) 5778-5788.

For 820 K and lower, and pressures lower than 1 bar:

$$k = 1.1 \times 10^{14} \text{ [cm}^3\text{/mol/s]}.$$

This study includes determinations of the rate of $\text{HCO} + \text{HCO}$ and $\text{HCO} + \text{M}$ also.

$\text{HCO} + \text{HCO} = \text{CH}_2\text{O} + \text{CO}$

G. Friedrichs, J. T. Herbon, D. F. Davidson, R. K. Hanson, "Quantitative Detection of HCO behind Shock Waves: The Thermal Decomposition of HCO ," Physical Chemistry Chemical Physics 4 (2002) 5778-5788.

For 820 K and lower, and pressures lower than 1 bar:

$$k = 2.7 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

This study includes determinations of the rate of $\text{H} + \text{HCO}$ and $\text{HCO} + \text{M}$ also.

$\text{H} + \text{CH}_2\text{O} = \text{H}_2 + \text{HCO}$

G. Friedrichs, D. F. Davidson, R. K. Hanson, "Direct Measurements of the Reaction of $\text{H} + \text{CH}_2\text{O} = \text{H}_2 + \text{HCO}$ Behind Shock Waves by Means of Vis-UV (correction V-UV) Detection of Formaldehyde," International Journal of Chemical Kinetics 34 (2002) 374-386.

For 1510-1969 K, 1.3 atm:

$$k = 6.6 \times 10^{14} \exp(-9313/RT) \text{ [cm}^3\text{/mol/s]}.$$

Title correction: July 18, 2002.

$\text{NH}_2 + \text{NO} = \text{Products}$

S. Song, R. K. Hanson, C. T. Bowman, D. M. Golden, "A Shock Tube Study of the Product Branching Ratio of the $\text{NH}_2 + \text{NO}$ Reaction at High Temperatures," Journal Physical Chemistry A 106 (2002) 9233-9235.

For 1826-2159 K, 1.10-1.21 bar:

Table of branching ratio data provided for $\text{NNH} + \text{OH}$ and $\text{N}_2 + \text{H}_2\text{O}$ channels.

$\text{NH}_2 + \text{NO}_2 = \text{Products}$

S. Song, D. M. Golden, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the $\text{NH}_2 + \text{NO}_2$ Reaction," Proceedings of the Combustion Institute 29 (2002) 2163-2170.

For 1330-1527 K, 1.31-1.49 bar:

$k = 5.5 \times 10^{12} \text{ [cm}^3/\text{mol/s]}$.

A branching ratio to the $\text{N}_2\text{O} + \text{H}_2\text{O}$ channel is also provided.

$\text{NH}_2 + \text{NO} = \text{Products}$

S. Song, R. K. Hanson, C. T. Bowman, D. M. Golden, "Shock Tube Determination of the Overall Rate of $\text{NH}_2 + \text{NO} = \text{Products}$ in the Thermal De-Nox Temperature Window," International Journal of Chemical Kinetics 33 (2001) 715-721. See also 2nd Joint Meeting of the U.S. Section of the Combustion Institute, Oakland CA, March 25-28, 2001, Paper 204.

For 1262-1726 K, 1.14-1.44 bar:

$k = 6.83 \times 10^{15} T^{-1.203} \exp(211/RT) \text{ [cm}^3/\text{mol/s]}$.

This reaction rate determination combines the data from this study and our previous higher temperature study S. Song, R. K. Hanson, C. T. Bowman, D. M. Golden, Proc. Comb. Inst. 28 (2000) 2403-2409.

$\text{NH}_2 + \text{NO} = \text{Products}$

S. Song, R. K. Hanson, C. T. Bowman, D. M. Golden, "Shock Tube Determination of the Overall Rate of $\text{NH}_2 + \text{NO} = \text{Products}$ at High Temperatures," Proceedings of the Combustion Institute 28 (2000) 2403-2409.

For 1716-2507 K, 1.0-1.38 bar:

$k = 2.08 \times 10^{16} T^{-1.34} \text{ [cm}^3/\text{mol/s]}$.

A lower temperature study of this reaction rate was also performed: S. Song, R. K. Hanson, C. T. Bowman, D. M. Golden, Internat. J. Chem. Kinet. 33 (2001) 715-721.

1995-1999

NH₂ + NO = Products

M. Votsmeier, S. Song, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Product Branching Ratio for the Reaction $\text{NH}_2 + \text{NO}$ Using Frequency-Modulation Detection of NH_2 ," Journal Physical Chemistry A 103 (1999) 1566-1571.

For 1340-1670 K, 1.3 atm:

Table of branching ratio data provided for $\text{NNH} + \text{OH}$ and $\text{N}_2 + \text{H}_2\text{O}$ channels.

CH + O₂ = Products

M. Roehrig, E. L. Petersen, D. F. Davidson, R. K. Hanson, C. T. Bowman, "Measurement of the Rate Coefficient of the Reaction $\text{CH} + \text{O}_2 = \text{Products}$ in the Temperature Range 2200 to 2600 K," International Journal of Chemical Kinetics 29 (1997) 781-789.

For 2200-2600 K, 1.3 atm:

$k = 9.77 \times 10^{13} \text{ [cm}^3/\text{mol/s]}$.

This study also includes a determination of the rate of $\text{CH}_3 + \text{M}$ and $\text{CH}_2 + \text{H}$.

CH₂ + H = CH + H₂

M. Roehrig, E. L. Petersen, D. F. Davidson, R. K. Hanson, C. T. Bowman, "Measurement of the Rate Coefficient of the Reaction $\text{CH} + \text{O}_2 = \text{Products}$ in the Temperature Range 2200 to 2600 K," International Journal of Chemical Kinetics 29 (1997) 781-789.

For 2200-2600 K, 1.3 atm:

$k = 1.41 \times 10^{14} \text{ [cm}^3/\text{mol/s]}$.

This study also includes a determination of the rate of $\text{CH}_3 + \text{M}$ and $\text{CH} + \text{O}_2$.

NO₂ + NO₂ = Products

M. Roehrig, E. L. Petersen, D. F. Davidson, R. K. Hanson, "A Shock Tube Study of the Pyrolysis of NO_2 ," International Journal of Chemical Kinetics 29 (1997) 483-493.

For 1350-2100 K, 42-380 atm:

$k = 2.00 \times 10^{12} \exp(-25120/\text{RT}) \text{ [cm}^3/\text{mol/s]}$ for the $2\text{NO} + \text{O}_2$ channel;

$k = 1.00 \times 10^{13} \exp(-25837/\text{RT}) \text{ [cm}^3/\text{mol/s]}$ for the $\text{NO}_3 + \text{NO}$ channel.

This study also includes a determination of the reaction rate of $\text{NO}_2 + \text{M}$.

CH₃ + CH₃ = Products

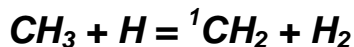
D. F. Davidson, M. D. Di Rosa, E. J. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Methyl-Methyl Reactions between 1200 and 2400 K," International Journal of Chemical Kinetics 27 (1995) 1179-1196.

For 1570-1780 K, 0.46-1.52 atm:

$k = 2.4 \times 10^{13} \exp(-12875/\text{RT}) \text{ [cm}^3/\text{mol/s]}$ for the $\text{C}_2\text{H}_5 + \text{H}$ channel.

k is less than $1 \times 10^{11} \text{ [cm}^3/\text{mol/s]}$ for the $\text{C}_2\text{H}_4 + \text{H}_2$ channel.

This paper also provides a reaction rate for $\text{CH}_3 + \text{H}$.

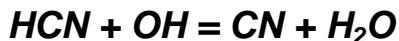


D. F. Davidson, M. D. Di Rosa, E. J. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Methyl-Methyl Reactions between 1200 and 2400 K," International Journal of Chemical Kinetics 27 (1995) 1179-1196.

For 1800-2200 K, 1.79-2.20 atm:

$k = 1.3 \times 10^{14} \text{ [cm}^3\text{/mol/s]}$ for the reverse reaction rate ${}^1\text{CH}_3 + \text{H}_2 = \text{CH}_3 + \text{H}$.

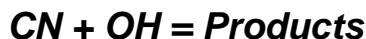
This paper also provides a reaction rate for $\text{CH}_3 + \text{CH}_3 = \text{Products}$.



S. T. Wooldridge, R. K. Hanson, C. T. Bowman, "Simultaneous Laser Absorption Measurements of $\text{CN} + \text{OH}$ in a Shock Tube Study of $\text{HCN} + \text{OH} = \text{Products}$," International Journal of Chemical Kinetics 27 (1995) 1075-1087.

For 1120-1960 K, 0.15-1.01 atm:

$k = 3.90 \times 10^6 T^{1.83} \exp(-10290/RT) \text{ [cm}^3\text{/mol/s]}$.



S. T. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of CN with HCN , OH and H_2 using CN and OH Laser Absorption," International Journal of Chemical Kinetics 28 (1996) 245-258.

For 1250-1860 K, 0.19-0.35 atm:

$k = 4.0 \times 10^{13} \text{ [cm}^3\text{/mol/s]}$.

This study also includes reaction rates for $\text{CN} + \text{HCN}$ and $\text{CN} + \text{H}_2$.

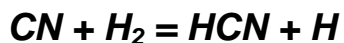


S. T. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of CN with HCN , OH and H_2 using CN and OH Laser Absorption," International Journal of Chemical Kinetics 28 (1996) 245-258.

For 940-1860 K, 0.19-0.35 atm:

$k = 1.51 \times 10^7 T^{1.71} \exp(-1530/RT) \text{ [cm}^3\text{/mol/s]}$ (reaction rate of D. L. Yang, T. Yu, M. C. Lin, C. F. Melius, J. Chem. Phys. 97 (1992) 222.)

This study also includes reaction rates for $\text{CN} + \text{OH}$ and $\text{CN} + \text{H}_2$.



S. T. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of CN with HCN , OH and H_2 using CN and OH Laser Absorption," International Journal of Chemical Kinetics 28 (1996) 245-258.

For 940-1860 K, 0.19-0.35 atm:

$k = 2.95 \times 10^5 T^{2.45} \exp(-2237/RT) \text{ [cm}^3\text{/mol/s]}$.

This study also includes reaction rates for $\text{CN} + \text{HCN}$ and $\text{CN} + \text{OH}$.

CN + H₂ = HCN + H

S. T. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of CN with HCN, OH and H₂ using CN and OH Laser Absorption," International Journal of Chemical Kinetics 28 (1996) 245-258.

For 940-1860 K, 0.19-0.35 atm:

$$k = 2.95 \times 10^5 T^{2.45} \exp(-2237/RT) \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for CN+HCN and CN+OH.

HNCO + OH = Products

M. S. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of CO+OH=CO₂+H and HNCO+OH=Products via Simultaneous Laser Absorption Measurements of OH and CO₂," International Journal of Chemical Kinetics 28 (1996) 361-372.

For 620-1860 K, 0.149-0.247 atm:

$$k = 3.63 \times 10^7 T^{1.5} \exp(-3594/RT) \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for CO+OH.

CO + OH = CO₂ + H

M. S. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of CO+OH=CO₂+H and HNCO+OH=Products via Simultaneous Laser Absorption Measurements of OH and CO₂," International Journal of Chemical Kinetics 28 (1996) 361-372.

For 1155-1432 K, 0.243-0.490 atm:

$$k = 2.12 \times 10^{12} \exp(-5226/RT) \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for HNCO+OH.

1990-1994

CN + NO₂ = Products

S. T. Wooldridge, J. D. Mertens, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of CN and NCO with NO₂," Proceedings of the Combustion Institute 25 (1994) 983-991. See also Western States Section/The Combustion Institute 1993 Fall Meeting, Menlo Park CA, October 18-19, 1993, paper 93-111.

For 1000-1600 K, 1.4 atm:

$$k = 1.59 \times 10^{13} \exp(-1133/RT) \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for NCO+NO₂.

NCO + NO₂ = Products

S. T. Wooldridge, J. D. Mertens, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of CN and NCO with NO₂," Proceedings of the Combustion Institute 25 (1994) 983-991. See also Western States Section/The Combustion Institute 1993 Fall Meeting, Menlo Park CA, October 18-19, 1993, paper 93-111.

For 1250 K, 1.4 atm:

$$k = 4.5 \times 10^{12} \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for CN+NO₂.

H + O₂ = OH + O

C.-L. Yu, M. Frenklach, D. A. Masten, R. K. Hanson, C. T. Bowman, "Reexamination of Shock Tube Measurements of the Rate Coefficient of H+O₂=OH+O," Journal Physical Chemistry 98 (1994) 4770-4771.

For 1800-2500 K, 1.4 atm:

$$k = 8.3 \times 10^{13} \exp(-14425/RT) \text{ [cm}^3\text{/mol/s]}.$$

This is a review article.

CO + OH = CO₂ + H

M. S. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the CO+OH=CO₂+H Reaction," Proceedings of the Combustion Institute 25 (1994) 741-748.

For 1090-2370 K, 0.19-0.82 atm:

$$k = 2.12 \times 10^{12} \exp(-5226/RT) \text{ [cm}^3\text{/mol/s]}.$$

OH + OH = H₂O + O

M. S. Wooldridge, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the OH+OH=H₂O+O Reaction," International Journal of Chemical Kinetics 26 (1994) 389-401. See also Western States Section/The Combustion Institute 1992 Fall Meeting, Berkeley CA, October 12-13, 1992, paper 92-93.

For 1050-2380 K, 0.18-0.60 atm:

$$k = 9.40 \times 10^{-5} T^{4.77} \exp(-9080/RT) \text{ [cm}^3\text{/mol/s]}.$$

O + HNCO = Products

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Reactions of Atomic Oxygen with Isocyanic Acid," International Journal of Chemical Kinetics 24 (1992) 279-295.

For 2120-3190 K, 0.25-1.11 atm:

$k = 1.9 \times 10^{13} \exp(-14207/RT)$ [cm³/mol/s] for the NH+CO₂ channel.

$k = 1.4 \times 10^{14} \exp(-20466/RT)$ [cm³/mol/s] for the OH+NCO channel.

This study also includes reaction rates for HNCO+OH.

OH + HNCO = Products

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of Reactions of Atomic Oxygen with Isocyanic Acid," International Journal of Chemical Kinetics 24 (1992) 279-295.

For 2120-2350 K, 0.25-1.11 atm:

An upper limit for this rate was determined to be $k = 1.5 \times 10^{12}$ [cm³/mol/s].

This study also includes reaction rates for HNCO+O.

C(³P) + H₂ = CH + H

A. J. Dean, D. F. Davidson, R. K. Hanson, "A Shock Tube Study of Reactions of C Atoms with H₂ and O₂ using Excimer Photolysis of C₃O₂ and C Atom Atomic Resonance Absorption Spectroscopy," Journal Physical Chemistry 95 (1991) 183-191.

For 1504-2042 K, 0.61-0.83 atm:

$k = 4.0 \times 10^{14} \exp(-23247/RT)$ [cm³/mol/s].

This study also includes rates for C+O₂ and C+C₃O₂.

C(³P) + O₂ = CO + O

A. J. Dean, D. F. Davidson, R. K. Hanson, "A Shock Tube Study of Reactions of C Atoms with H₂ and O₂ using Excimer Photolysis of C₃O₂ and C Atom Atomic Resonance Absorption Spectroscopy," Journal Physical Chemistry 95 (1991) 183-191.

For 1517-4185 K, 0.64-1.21 atm:

$k = 1.2 \times 10^{14} \exp(-3994/RT)$ [cm³/mol/s].

This study also includes rates for C+H₂ and C+C₃O₂.

C(³P) + C₃O₂ = Products

A. J. Dean, D. F. Davidson, R. K. Hanson, "A Shock Tube Study of Reactions of C Atoms with H₂ and O₂ using Excimer Photolysis of C₃O₂ and C Atom Atomic Resonance Absorption Spectroscopy," Journal Physical Chemistry 95 (1991) 183-191.

For 1450-1900 K, 0.6-1.2 atm:

$k = 2.4 \times 10^{19} T^{-1.75}$ [cm³/mol/s].

This study also includes rates for C+O₂ and C+H₂.

CN + O = CO + N

D. F. Davidson, A. J. Dean, M. D. DiRosa, R. K. Hanson, C. T. Bowman, "*Shock Tube Measurements of the Reactions of CN with O and O₂*," International Journal of Chemical Kinetics 23 (1991) 1035-1050. See also The Combustion Institute/Western States Section 1990 Fall Meeting, La Jolla CA, October 15-16, 1990, Paper 90-13.

For 3000-4500 K, 0.45-0.90 atm:

$$k = 7.7 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for CN+O₂.

CN + O₂ = NCO + O

D. F. Davidson, A. J. Dean, M. D. DiRosa, R. K. Hanson, C. T. Bowman, "*Shock Tube Measurements of the Reactions of CN with O and O₂*," International Journal of Chemical Kinetics 23 (1991) 1035-1050. See also The Combustion Institute/Western States Section 1990 Fall Meeting, La Jolla CA, October 15-16, 1990, Paper 90-13.

For 2700-3800 K, 0.62-1.05 atm:

$$k = 1.0 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

This study also includes reaction rates for CN+O.

N₂O + O = Products

D. F. Davidson, M. D. DiRosa, A. Y. Chang, R. K. Hanson, "*Shock Tube Measurements of the Major Product Channels of N₂O+O*," Proceedings of the 18th International Symposium on Shock Waves, Sendai, Japan, July 21-26, 1991, pp. 813-818.

For 1680-3340 K, 0.7-2.0 atm:

$$k = 2.9 \times 10^{13} \exp(-23149/RT) \text{ [cm}^3\text{/mol/s]} \text{ for the NO+NO channel.}$$

$$k = 1.4 \times 10^{12} \exp(-10809/RT) \text{ [cm}^3\text{/mol/s]} \text{ for the N}_2\text{+O}_2 \text{ channel.}$$

C(³P) + NO = Products

A. J. Dean, R. K. Hanson, C. T. Bowman, "*A Shock Tube Study of Reactions of C Atoms and CH with NO including Product Channel Measurements*," Journal Physical Chemistry 95 (1991) 3180-3189.

For 1550-4050 K, 0.5-1.0 atm:

$$k = 4.8 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

This study also includes branching ratio data for the two product channels CH+O and CO+N, and a determination of the CH+NO rate.

CH + NO = Products

A. J. Dean, R. K. Hanson, C. T. Bowman, "*A Shock Tube Study of Reactions of C Atoms and CH with NO including Product Channel Measurements*," Journal Physical Chemistry 95 (1991) 3180-3189.

For 1550-4050 K, 0.5-1.0 atm:

$$k = 1.0 \times 10^{14} \text{ [cm}^3\text{/mol/s]}.$$

This study also includes branching ratio data for the three product channels including HCN+O, NH+CO and OH+CN, and a determination of the C+NO rate.

H + HNCO = NH₂ + CO

J. D. Mertens, K. Kohse-Hoeinghaus, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of $H+HNCO=NH_2+CO$," International Journal of Chemical Kinetics 23 (1991) 655-668.

For 2340-3270 K, 0.33-0.49 atm:

$$k = 2.1 \times 10^{14} \exp(-16889/RT) \text{ [cm}^3\text{/mol/s]}.$$

An upper limit for NH₂+HNCO is also included in this paper.

NH₂ + HNCO = NH₃ + NCO

J. D. Mertens, K. Kohse-Hoeinghaus, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of $H+HNCO=NH_2+CO$," International Journal of Chemical Kinetics 23 (1991) 655-668.

For 2340-2680 K, 0.33-0.49 atm:

$$\text{Upper limit for } k = 5.0 \times 10^{11} \text{ [cm}^3\text{/mol/s]}.$$

A reaction rate for H+HNCO is also included in this paper.

NH + NO = Products

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of NH with NO, O₂ and O," International Journal of Chemical Kinetics 23 (1991) 173-196. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-96.

For 2220-3350 K, 0.1-1.0 atm:

$$k = 1.7 \times 10^{14} \exp(-12716/RT) \text{ [cm}^3\text{/mol/s]}.$$

Reaction rates for NH+O₂ and NH+O are also included in this paper.

NH + O₂ = Products

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of NH with NO, O₂ and O," International Journal of Chemical Kinetics 23 (1991) 173-196. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-96.

For 2220-3350 K, 0.1-1.0 atm:

$$k = 3.5 \times 10^{13} \exp(-17088/RT) \text{ [cm}^3\text{/mol/s]}.$$

Reaction rates for NH+NO and NH+O are also included in this paper.

NH + O = Products

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "A Shock Tube Study of the Reactions of NH with NO, O₂ and O," International Journal of Chemical Kinetics 23 (1991) 173-196. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-96.

For 2220-3350 K, 0.1-1.0 atm:

$$k = 9.2 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

Reaction rates for NH+O₂ and NH+NO are also included in this paper.

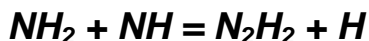


D. F. Davidson, K. Kohse-Hoeinghaus, A. Y. Chang, R. K. Hanson, , "A Pyrolysis Mechanism for Ammonia," International Journal of Chemical Kinetics 22 (1990) 513-535. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-95.

For 2200-2800 K, 0.8-1.1 atm:

$$k = 4.0 \times 10^{13} \exp(-7252/RT) [\text{cm}^3/\text{mol/s}].$$

Reaction rates for $\text{NH}_2 + \text{NH}$, $\text{NH}_2 + \text{NH}_2$ and $\text{NH}_3 + \text{M}$ are also included in this paper.

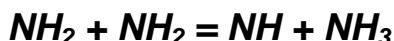


D. F. Davidson, K. Kohse-Hoeinghaus, A. Y. Chang, R. K. Hanson, , "A Pyrolysis Mechanism for Ammonia," International Journal of Chemical Kinetics 22 (1990) 513-535. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-95.

For 2200-2800 K, 0.8-1.1 atm:

$$k = 1.5 \times 10^{15} T^{-0.5} [\text{cm}^3/\text{mol/s}].$$

Reaction rates for $\text{NH}_2 + \text{H}$, $\text{NH}_2 + \text{NH}_2$ and $\text{NH}_3 + \text{M}$ are also included in this paper.



D. F. Davidson, K. Kohse-Hoeinghaus, A. Y. Chang, R. K. Hanson, , "A Pyrolysis Mechanism for Ammonia," International Journal of Chemical Kinetics 22 (1990) 513-535. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-95.

For 2200-2800 K, 0.8-1.1 atm:

$$k = 5.0 \times 10^{13} \exp(-19870/RT) [\text{cm}^3/\text{mol/s}].$$

Reaction rates for $\text{NH}_2 + \text{NH}$, $\text{NH}_2 + \text{H}_2$ and $\text{NH}_3 + \text{M}$ are also included in this paper.

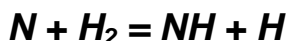


D. F. Davidson, R. K. Hanson, , "High Temperature Reaction Rate Coefficients Derived from N-ARAS Measurements and Excimer Photolysis of NO," International Journal of Chemical Kinetics 22 (1990) 843-861. See also AIP Conference Proceedings 208, 17th International Symposium on Shock Waves and Shock Tubes, Bethlehem PA 1989, pp. 525-530.

For 1400-3500 K, 0.6 atm:

$$k = 4.29 \times 10^{13} \exp(-1564/RT) [\text{cm}^3/\text{mol/s}].$$

A reaction rate for $\text{N} + \text{H}_2$ is also included in this paper.

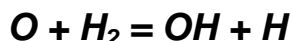


D. F. Davidson, R. K. Hanson, , "High Temperature Reaction Rate Coefficients Derived from N-ARAS Measurements and Excimer Photolysis of NO," International Journal of Chemical Kinetics 22 (1990) 843-861. See also AIP Conference Proceedings 208, 17th International Symposium on Shock Waves and Shock Tubes, Bethlehem PA 1989, pp. 525-530.

For 1400-3500 K, 0.6 atm:

$k = 1.60 \times 10^{14} \exp(-63663/RT) \text{ [cm}^3/\text{mol/s]}$.

A reaction rate for N+NO is also included in this paper.



D. F. Davidson, R. K. Hanson, "A Direct Comparison of Shock Tube Photolysis and Pyrolysis Methods in the Determination of the Rate Coefficient for $O+H_2=OH+H$," Combustion and Flame 82 (1990) 445-447.

For 2120-2750 K, 0.5 atm:

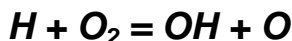
$k = 8.13 \times 10^{14} \exp(-18955/RT) \text{ [cm}^3/\text{mol/s]}$.



D. F. Davidson, R. K. Hanson, "Shock Tube Measurements of the Rate Coefficient for $N+CH_3=H_2CN+H$ using N-Atom ARAS and Excimer Photolysis of NO," Proceedings of the Combustion Institute 23 (1990) 267-273.

For 1600-2000 K, 0.5 atm:

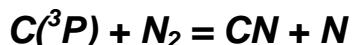
$k = 7.1 \times 10^{13} \text{ [cm}^3/\text{mol/s]}$.



D. A. Mastern, R. K. Hanson, C. T. Bowman, "Shock Tube Study of the Reaction of $H+O_2=OH+O$ Using OH Laser Absorption," Journal Physical Chemistry 94 (1990) 7119-7128. See also Western States Section/ The Combustion Institute 1989 Fall Meeting, Livermore CA October 23-24, 1989, Paper 89-97.

For 1450-3370 K, 0.35-2.5 atm:

$k = 9.33 \times 10^{13} \exp(-14800/RT) \text{ [cm}^3/\text{mol/s]}$.



A. J. Dean, R. K. Hanson, C. T. Bowman, "High Temperature Shock Tube Study of Reactions of CH and C-Atoms with N_2 ," Proceedings of the Combustion Institute 23 (1990) 267-273.

For 2660-4660 K, 0.5-1.0 atm:

$k = 6.3 \times 10^{13} \exp(-46018/RT) \text{ [cm}^3/\text{mol/s]}$.

This paper includes a rate for CH+N2 as well.



A. J. Dean, R. K. Hanson, C. T. Bowman, "High Temperature Shock Tube Study of Reactions of CH and C-Atoms with N_2 ," Proceedings of the Combustion Institute 23 (1990) 267-273.

For 2500-3800 K, 0.6-1.0 atm:

$k = 4.4 \times 10^{12} \exp(-21976/RT) \text{ [cm}^3/\text{mol/s]}$.

This paper includes a rate for CH+N2 as well.

1986-1989

NH + NH = Products

J. D. Mertens, A. Y. Chang, R. K. Hanson, C. T. Bowman, "*Reaction Kinetics of NH in the Shock Tube Pyrolysis of HNCO*," International Journal of Chemical Kinetics 21 (1989) 1049-1067. See also Western States Section/ The Combustion Institute 1988 Fall Meeting, Dana Point CA October 17-18, 1988, Paper 88-64.

For 2070-2730 K, 0.3-2.1 atm:

$$k = 5.1 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

This paper provides reaction rates for HNCO+M and NH+Ar as well.

H + H₂O = OH + H₂

D. F. Davidson, A. Y. Chang, R. K. Hanson, "*Laser Photolysis Shock Tube for Combustion Kinetics Studies*," Proceedings of the Combustion Institute 22 (1988) 1877-1885.

For 1600-2500 K, 1.2 atm:

$$k = 2.4 \times 10^{14} \exp(-21360/RT) \text{ [cm}^3\text{/mol/s]}.$$

1974-1985

$\text{NCO} + \text{H} = \text{NH} + \text{CO}$

M. Y. Louge, R. K. Hanson, "High Temperature Kinetics of NCO," Combustion and Flame 58 (1984) 291-300.

For 1490 K, 0.6 atm:

$$k = 5.37 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

Rates are also presented for NCO+M and NCO+H₂.

$\text{NCO} + \text{H}_2 = \text{HNCO} + \text{H}$

M. Y. Louge, R. K. Hanson, "High Temperature Kinetics of NCO," Combustion and Flame 58 (1984) 291-300.

For 1490 K, 0.6 atm:

$$k = 1.25 \times 10^{12} \text{ [cm}^3\text{/mol/s]}.$$

Rates are also presented for NCO+M and NCO+H.

$\text{CN} + \text{H}_2\text{O} = \text{HCN} + \text{OH}$

A. Szekely, R. K. Hanson, C. T. Bowman, "High Temperature Determination of the Rate Coefficient for the Reaction $\text{H}_2\text{O} + \text{CN} = \text{HCN} + \text{OH}$," International Journal of Chemical Kinetics 16 (1984) 1609-1621.

For 2460-2840 K, 0.4-0.6 atm:

$$k = 2.3 \times 10^{13} \exp(-13312/RT) \text{ [cm}^3\text{/mol/s]}.$$

$\text{C}_2\text{N}_2 + \text{O} = \text{CN} + \text{NCO}$

M. Louge, R. K. Hanson, "Shock Tube Study of Cyanogen Oxidation Kinetics," International Journal of Chemical Kinetics 16 (1984) 231-250.

For 2000 K, 0.6 atm:

$$k = 5.0 \times 10^{11} \text{ [cm}^3\text{/mol/s]}.$$

Rates are also presented for CN+O.

$\text{CN} + \text{O} = \text{CO} + \text{N}$

M. Louge, R. K. Hanson, "Shock Tube Study of Cyanogen Oxidation Kinetics," International Journal of Chemical Kinetics 16 (1984) 231-250.

For 2000 K, 0.6 atm:

$$k = 1.8 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

Rates are also presented for C₂N₂+O.

$\text{HCN} + \text{O} = \text{Products}$

A. Szekely, R. K. Hanson, C. T. Bowman, "Shock Tube Study of the Reaction between Hydrogen Cyanide and Atomic Oxygen," Proceedings of the Combustion Institute 20 (1984) 647-654.

For 1800-2600 K, 0.6 atm:

$$k = 2.2 \times 10^{13} \exp(-15379/RT) \text{ [cm}^3\text{/mol/s]} \text{ for the NH+CO channel.}$$

k is less than $5.0 \times 10^{13} \text{ [cm}^3\text{/mol/s]}$ for the CN+OH channel.

$\text{NCO} + \text{O} = \text{CO} + \text{NO}$

M. Y. Louge, R. K. Hanson, "Shock Tube Study of NCO Kinetics," Proceedings of the Combustion Institute 20 (1984) 665-672.

For 1450 K, 0.6 atm:

$$k = 5.63 \times 10^{13}$$

A rate for $\text{HCN} + \text{O}$ is also presented in this paper.

$\text{HCN} + \text{O} = \text{NCO} + \text{H}$

M. Y. Louge, R. K. Hanson, "Shock Tube Study of NCO Kinetics," Proceedings of the Combustion Institute 20 (1984) 665-672.

For 1440 K, 0.6 atm:

$$k = 5.01 \times 10^{11}$$

A rate for $\text{NCO} + \text{O}$ is also presented in this paper.

$\text{CN} + \text{H}_2 = \text{HCN} + \text{H}$

A. Szekely, R. K. Hanson, C. T. Bowman, "High Temperature Determination of the Rate Coefficient for the Reaction $\text{H}_2 + \text{CN} = \text{H} + \text{HCN}$," International Journal of Chemical Kinetics 15 (1983) 915-923.

For 2700-3500 K, 0.4-0.6 atm:

$$k = 7.5 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

$\text{CN} + \text{HCN} = \text{C}_2\text{N}_2 + \text{H}$

A. Szekely, R. K. Hanson, C. T. Bowman, "High Temperature Determination of the Rate Coefficient for the Reaction $\text{H}_2 + \text{CN} = \text{H} + \text{HCN}$," International Journal of Chemical Kinetics 15 (1983) 1237-1241.

For 2720-3070 K, 0.4-0.6 atm:

$$k = 1.0 \times 10^{13} \text{ [cm}^3\text{/mol/s]}.$$

$\text{NH}_2 + \text{NO} = \text{Products}$

T. R. Roose, R. K. Hanson, C. H. Kruger, "A Shock Tube Study of the Decomposition of NO in the Presence of NH_3 ," Proceedings of the Combustion Institute 18 (1981) 853-862.

For 1680-2850 K, 0.6 atm:

$$k = 3.0 \times 10^{13} \exp(-15697/RT) \text{ [cm}^3\text{/mol/s]} \text{ for all products.}$$

$$k = 7.0 \times 10^{13} \exp(-27818/RT) \text{ [cm}^3\text{/mol/s]} \text{ for the } \text{N}_2\text{O} + \text{H}_2 \text{ channel.}$$

Rates for $\text{NH} + \text{NO}$ are also provided in this paper.

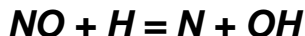
$\text{NH} + \text{NO} = \text{Products}$

T. R. Roose, R. K. Hanson, C. H. Kruger, "A Shock Tube Study of the Decomposition of NO in the Presence of NH_3 ," Proceedings of the Combustion Institute 18 (1981) 853-862. See also Proceedings of the 11th International Symposium on Shock Tubes and Waves (1978) pp. 245-253.

For 1760-2850 K, 0.6 atm:

$$k = 8.0 \times 10^{13} \exp(-29407/RT) \text{ [cm}^3\text{/mol/s]}.$$

Rates for $\text{NH}_2 + \text{NO}$ are also provided in this paper.



W. L. Flower, R. K. Hanson, C. H. Kruger, "Experimental Study of Nitric Oxide Decomposition by Reaction with Hydrogen," Combustion, Science and Technology 15 (1977) 115-128. See also the Proceedings of the Combustion Institute 15 (1975) 823-832.

For 2400-4200 K, 0.6 atm:

$$k = 2.22 \times 10^{14} \exp(-50500/RT) \text{ [cm}^3/\text{mol/s]}.$$



W. L. Flower, R. K. Hanson, C. H. Kruger, "Experimental Study of Nitric Oxide Decomposition by Reaction with Hydrogen," Combustion, Science and Technology 15 (1977) 115-128.

For 1815-3365 K, 0.6 atm:

$$k = 6.23 \times 10^{13} \exp(-24540/RT) \text{ [cm}^3/\text{mol/s]}.$$

A rate for $\text{N}_2\text{O} + \text{M}$ is also presented in this paper.



J. P. Monat, R. K. Hanson, C. H. Kruger, "Shock Tube Determination of the Rate Coefficient for the Reaction $\text{N}_2 + \text{O} = \text{NO} + \text{N}$," Proceedings of the Combustion Institute 15 (1975) 543-550.

For 2384-3850 K, 0.6 atm:

$$k = 1.84 \times 10^{14} \exp(-76250/RT) \text{ [cm}^3/\text{mol/s]}.$$



R. K. Hanson, W. L. Flower, C. H. Kruger, "Determination of the Rate Constant for the Reaction $\text{O} + \text{NO} = \text{N} + \text{O}_2$," Combustion Science and Technology 9 (1974) 79-86.

For 2500-4100 K, 0.6 atm:

$$k = 2.36 \times 10^9 T \exp(-38640/RT) \text{ [cm}^3/\text{mol/s]}.$$